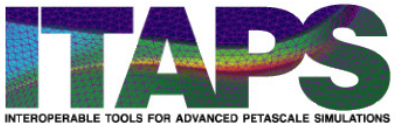
Adaptive Meshing Control to Improve Petascale Compass Simulations

Xiao-Juan Luo and Mark S Shephard

Scientific Computation Research Center (SCOREC)
Interoperable Technologies for Advanced Petascale Simulations Center (ITAPS)

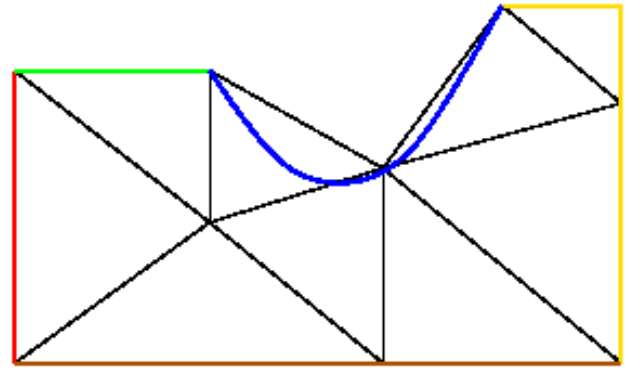
Lie-Quan Lee, Lixin Ge and Cho Ng

Stanford Linear Accelerator Center (SLAC)

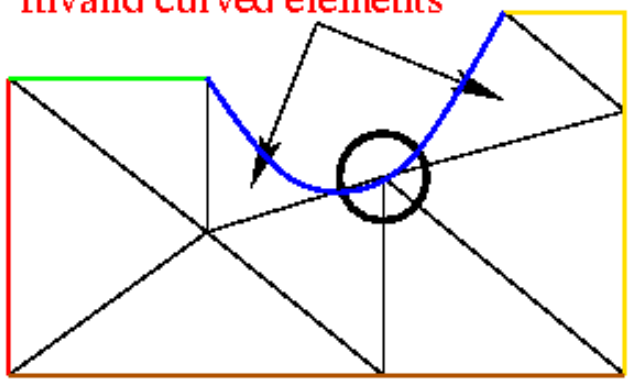


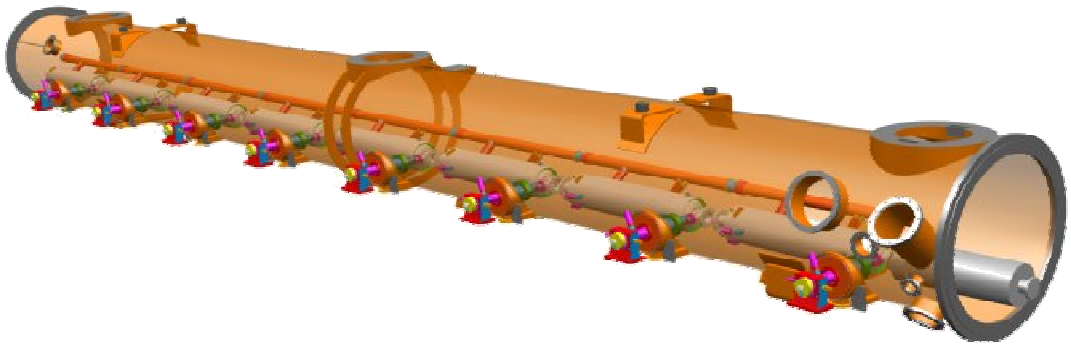
Motivations - Electromagnetic analysis

- Valid curvilinear meshes that properly satisfy the geometric approximation requirements
  - **Correct invalid curved elements due to mesh curving**
  - **Difficult to deal with 3D complex curved domains**



Invalid curved elements

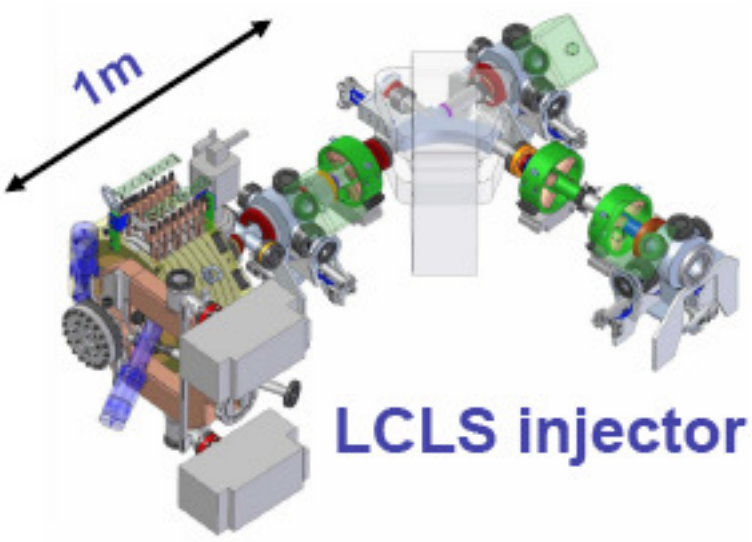




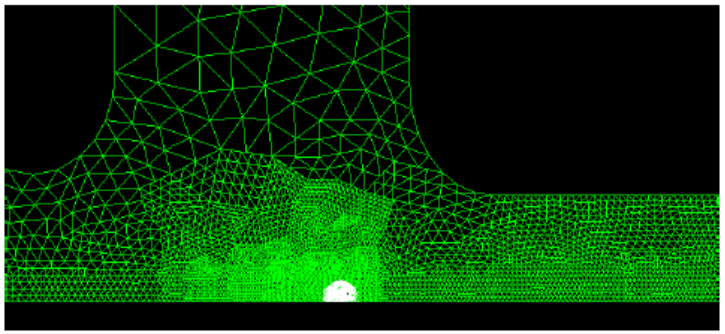
ILC cryomodule consisting of 8 TDR cavities

Motivations - Electromagnetic analysis

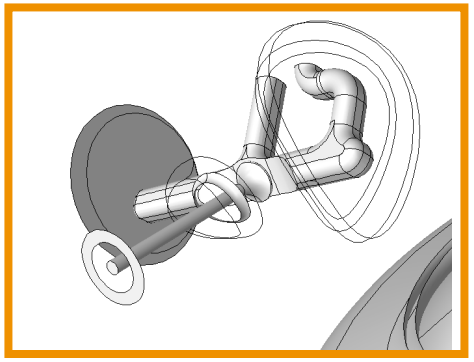
- Sufficiently refine the critical domains around the moving particle beams
  - **Resolve high frequency and improve computational efficiency**
  - **Move the refinement along with the particle beams**
  - **Smooth the mesh size between refine and coarse domains**
  - **Deal with 3D curved domains**



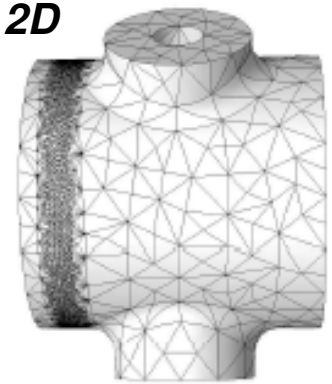
PIC in long structures



Adaptive refinement around the particle beam in 2D



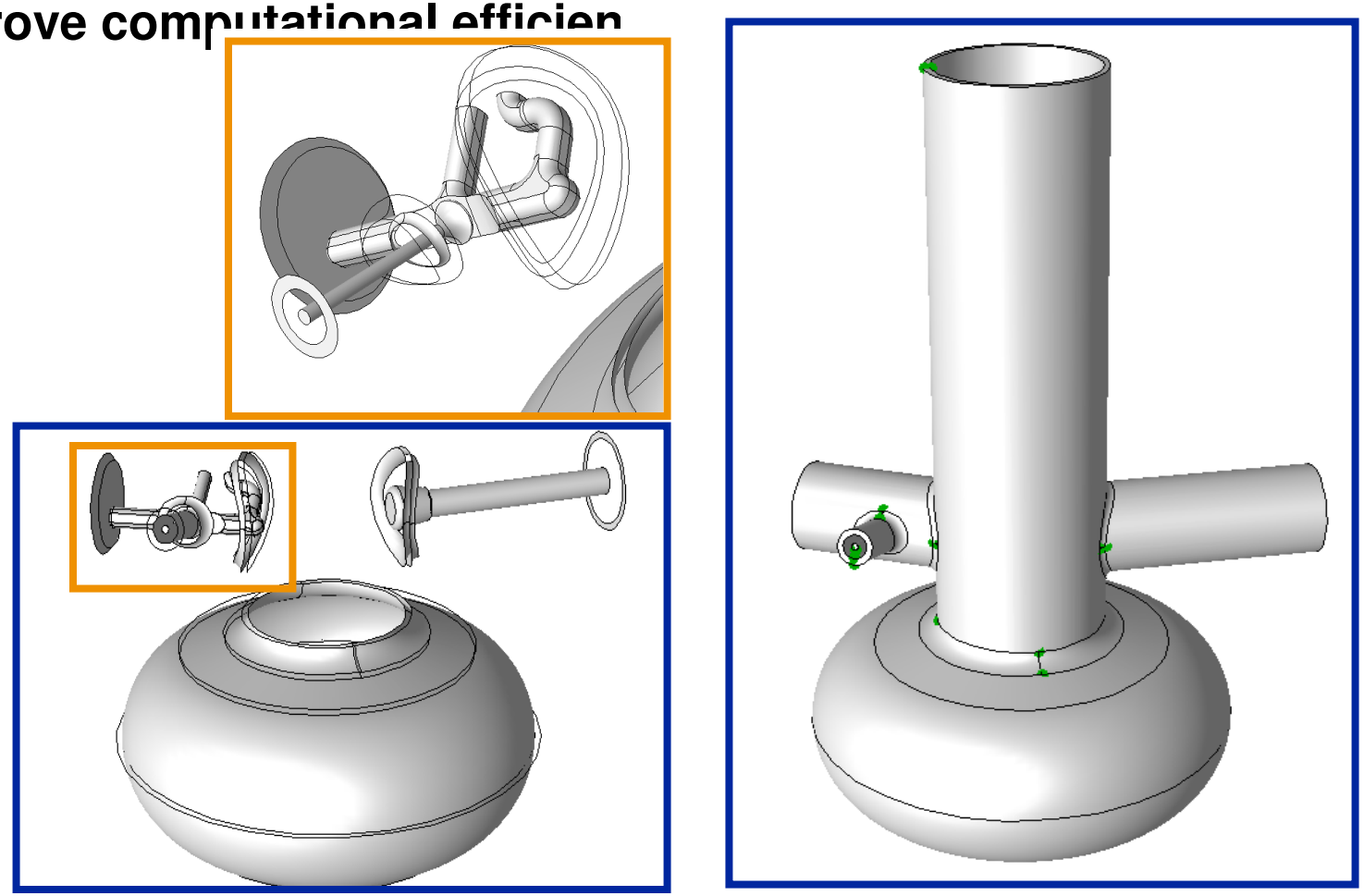
3D complex model



Unsmoothed size field

Motivations - Thermal/Mechanical Multiphysics Simulations

- Curved anisotropic meshes for thin sections
  - **Assign variable polynomial order at different directions**
  - **Improve computational efficien**



3D complex model with thin sections for thermal/mechanical multiphysics simulations

Correct Invalid Curved Elements

- Input
  - A Curved mesh with invalid regions
    - Generated by curving edges and faces of the straight-sided mesh on the model boundaries
    - The invalid regions created by incomplete method for curving elements
  - No model is needed
- Key steps and techniques
  - Apply Bezier high order mesh entity shape representation methods
  - Apply curved local mesh modifications to correct invalid regions
    - The surface geometric approximation remain unchanged if no model is provided
- Output
  - A correct curved mesh without any invalid regions

Curved Entity High-order Shape Representation

- Bezier bounding property to check the validity for curved regions

$$J = \left[\frac{\partial x_i^q}{\partial \xi_j}\right] = \begin{bmatrix} \frac{\partial x_1^q}{\partial \xi_1} & \frac{\partial x_1^q}{\partial \xi_2} & \frac{\partial x_1^q}{\partial \xi_3} \\ \frac{\partial x_2^q}{\partial \xi_1} & \frac{\partial x_2^q}{\partial \xi_2} & \frac{\partial x_2^q}{\partial \xi_3} \\ \frac{\partial x_3^q}{\partial \xi_1} & \frac{\partial x_3^q}{\partial \xi_2} & \frac{\partial x_3^q}{\partial \xi_3} \end{bmatrix} \qquad det(J) = (\frac{\partial \boldsymbol{x}^q}{\partial \xi_1} \times \frac{\partial \boldsymbol{x}^q}{\partial \xi_2}) \cdot (\frac{\partial \boldsymbol{x}^q}{\partial \xi_3})$$

$$det(J) = \sum_{|\boldsymbol{i}|=r} C_{|\boldsymbol{i}|}^r c_{|\boldsymbol{i}|}^r \boldsymbol{\xi}^{|\boldsymbol{i}|}$$

- $det(J)$ is also a Bezier function with order $3(q-1)$
- Bezier bounding property indicates that a curved region is valid globally if

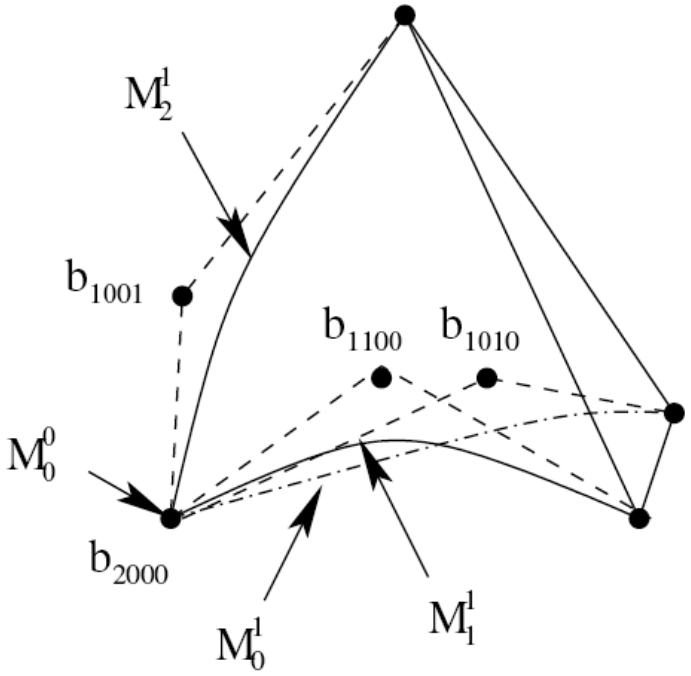
$$min(c_{|\boldsymbol{i}|}^r) \leq det(J) \leq max(c_{|\boldsymbol{i}|}^r)$$

Procedure to Correct Invalid Regions

- Put all of the invalid regions in a list
  - Each region has a list of key entities
- Traverse the list
  - Step 1. Apply operations other than reshape and refinement if possible
    - Termination: No operation can be executed or the list is empty.
  - Step 2. Recursively apply reshape
    - Termination: No reshape can be executed or the list is empty
  - Step 3. Refine the invalid regions and put the new created invalid regions in the list. Go to Step 1.
- The procedure ends when the list is empty

Determine Key Entities to Apply Modifications

- Determine the key entities for a invalid region
  - Compute the determinant of Jacobian
  - Check the negative coefficients $det(J) = \sum_{|\boldsymbol{i}|=r} C^r_{|\boldsymbol{i}|} c^r_{|\boldsymbol{i}|} \boldsymbol{\xi}^{|\boldsymbol{i}|}$
  - A negative corner coefficient corresponds to one vertex of the curved region, three edges and faces connected to the vertex are the candidates

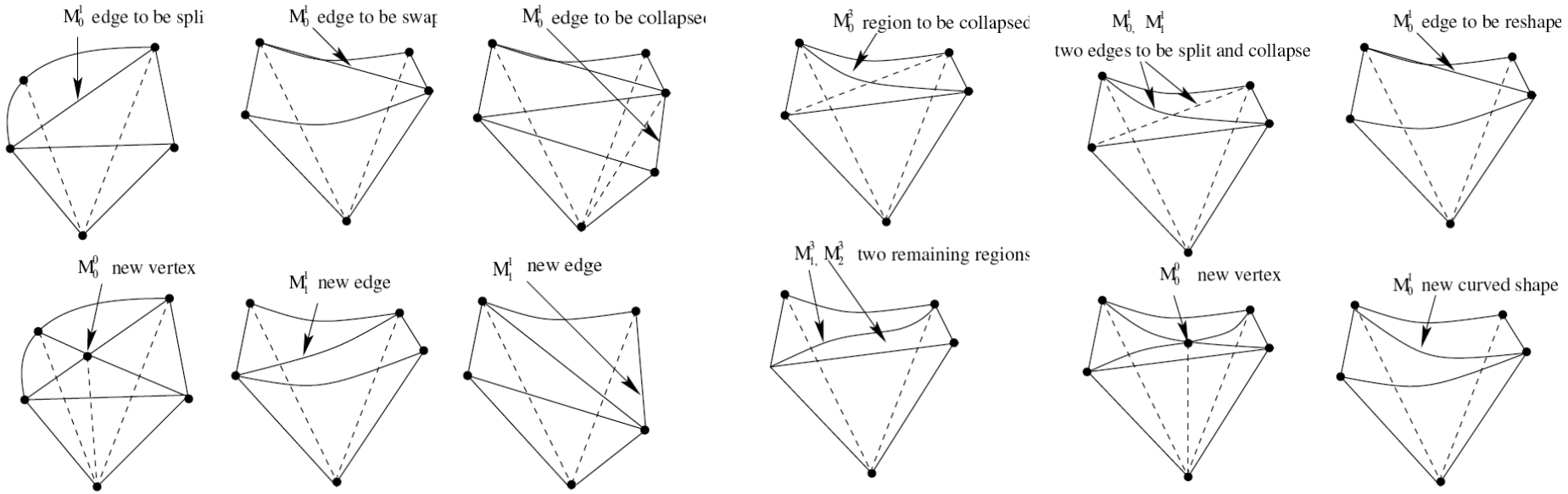


$$b_{2000} = (\vec{v}_0 \bullet \vec{v}_1) \times \vec{v}_2 < 0$$

$$M_0^0, M_0^1, M_1^1, M_2^1$$

Curved Local Mesh Modifications

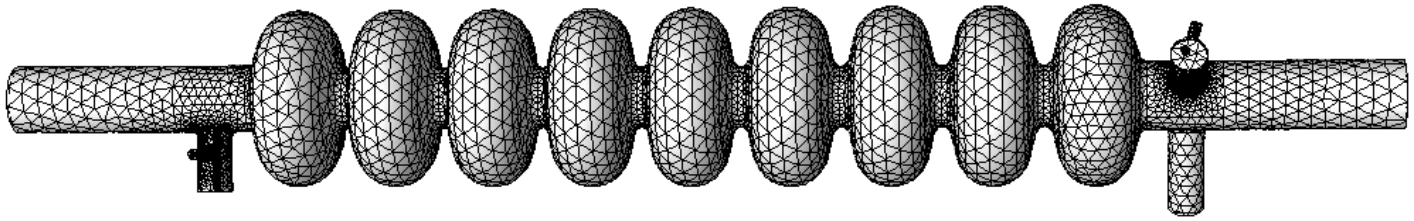
- Split, collapse, swap, split+collapse, reshape, and refinement to correct invalid mesh regions
  - Local cavity involves curved mesh entities - use curved validity check
  - Newly created entities must account for curved geometries

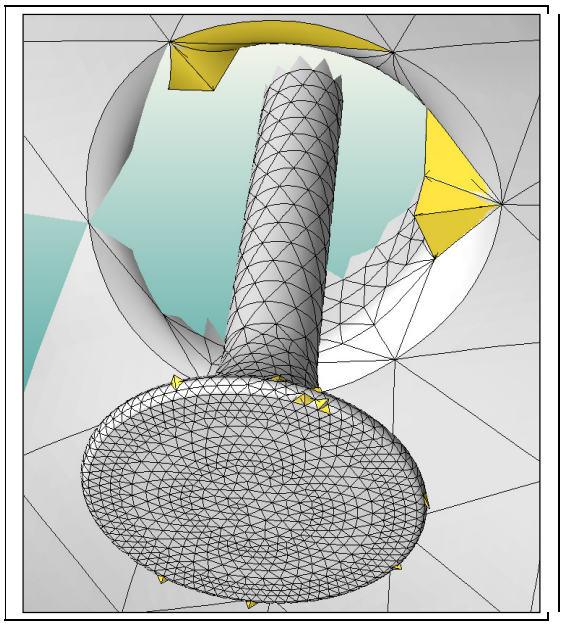


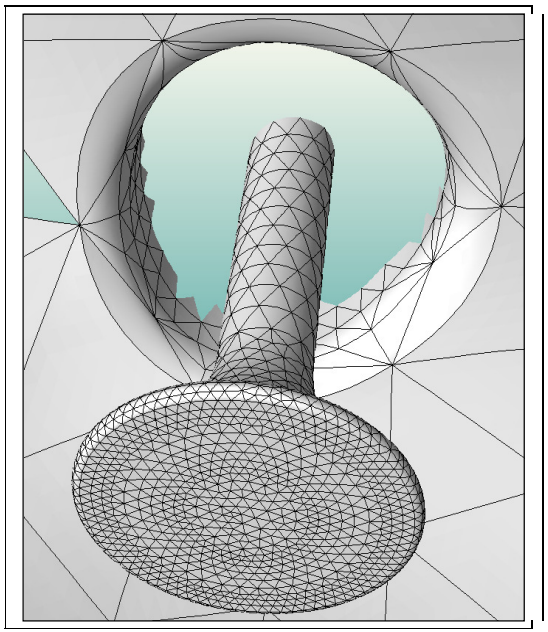
Demonstration

QuickTime™ and a
TIFF (Uncompressed) decompressor
are needed to see this picture.

Curved Mesh in 8-cavity Cryomodule Simulation



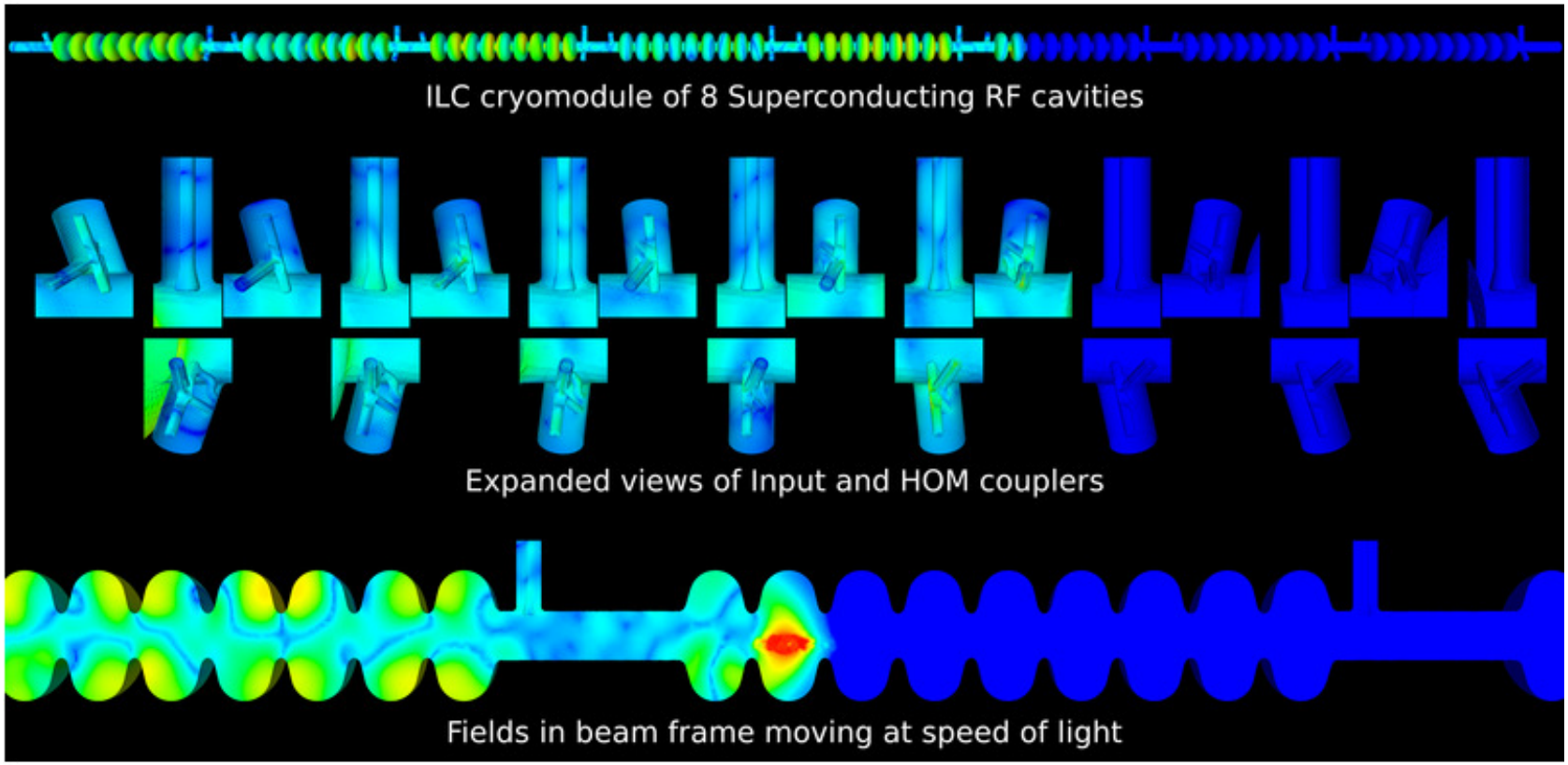




Edge collapse	253
Region collapse	17
Edge swap	76
Double edge split+collapse	13
Recurving	32

- **2.97** millions curved regions
- **515** invalid curved elements have been corrected

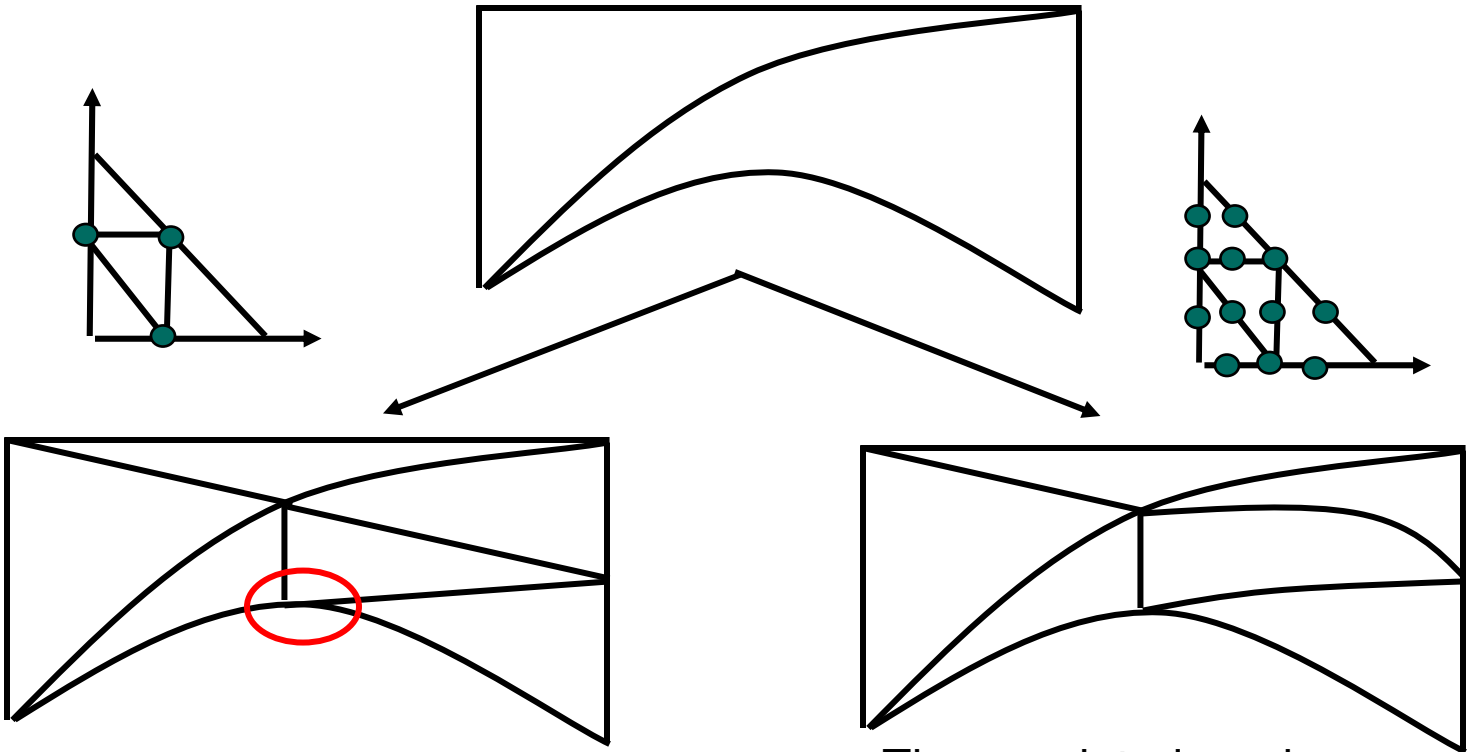
Curved Mesh in 8-cavity Cryomodule Simulation



- **20** million degree of freedoms. **256** multi-stream processors on Cray-X1E at Oak Ridge Nationl Laboratory and took **300** wall hours
- Execution time **30%** faster per time-step after correcting the invalid curved regions

Control of Moving Mesh Adaptation in Curved Domains

- Apply refinements on curved mesh entities



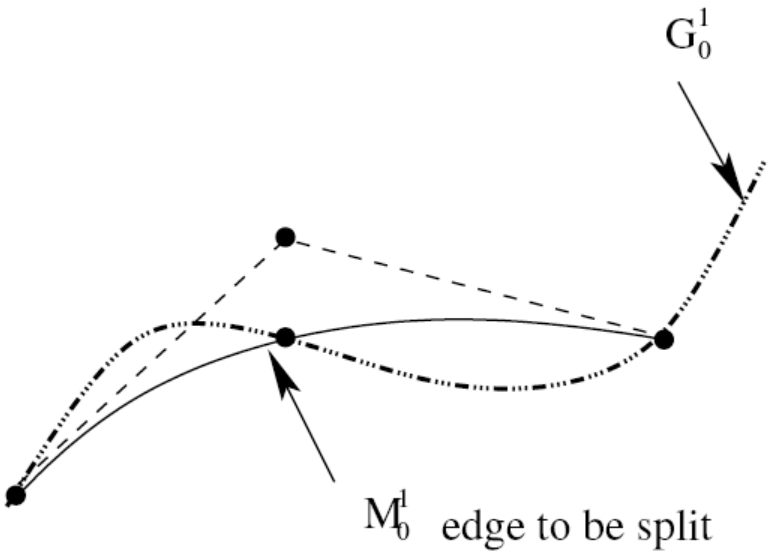
The new interior edges are straight-sided

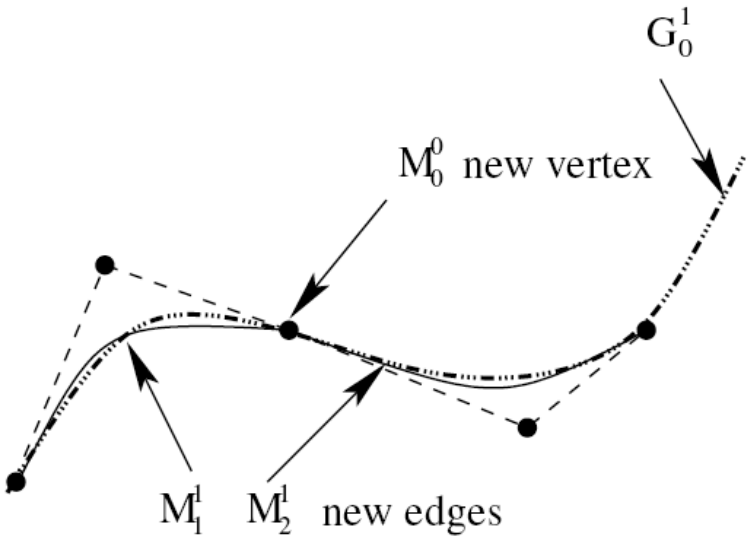
The new interior edges are determined based on the higher order split

Ensure the validity of a curved mesh after refinement

Control of Moving Mesh Adaptation in Curved Domains

- Curve newly created mesh entities to the boundaries
  - Curved validity check
  - Local mesh modifications to correct invalid elements





Control of Moving Mesh Adaptation in Curved Domains

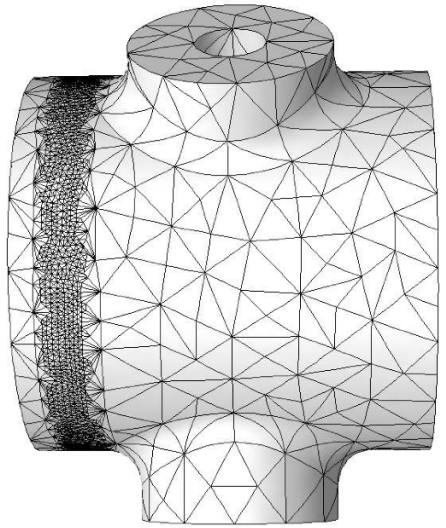
- Control mesh size gradation
  - The ratio between the larger mesh size to the smaller size at the two bounding mesh vertices of any mesh edges is under a prescribed factor (H. Borouchaki etc. 1998)

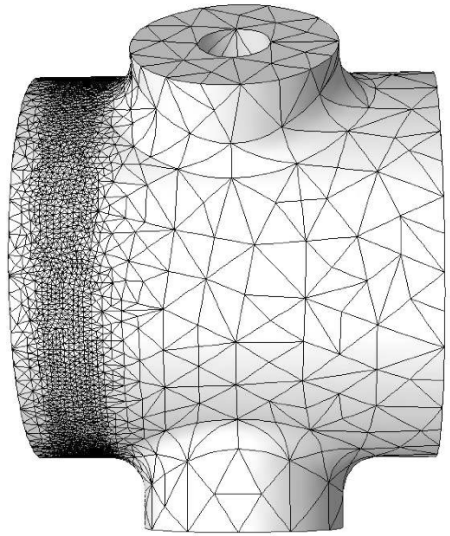
QuickTime™ and a
decompressor
are needed to see this picture.

QuickTime™ and a
decompressor
are needed to see this picture.

QuickTime™ and a
decompressor
are needed to see this picture.

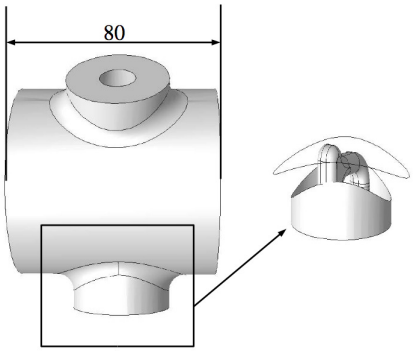
QuickTime™ and a
decompressor
are needed to see this picture.

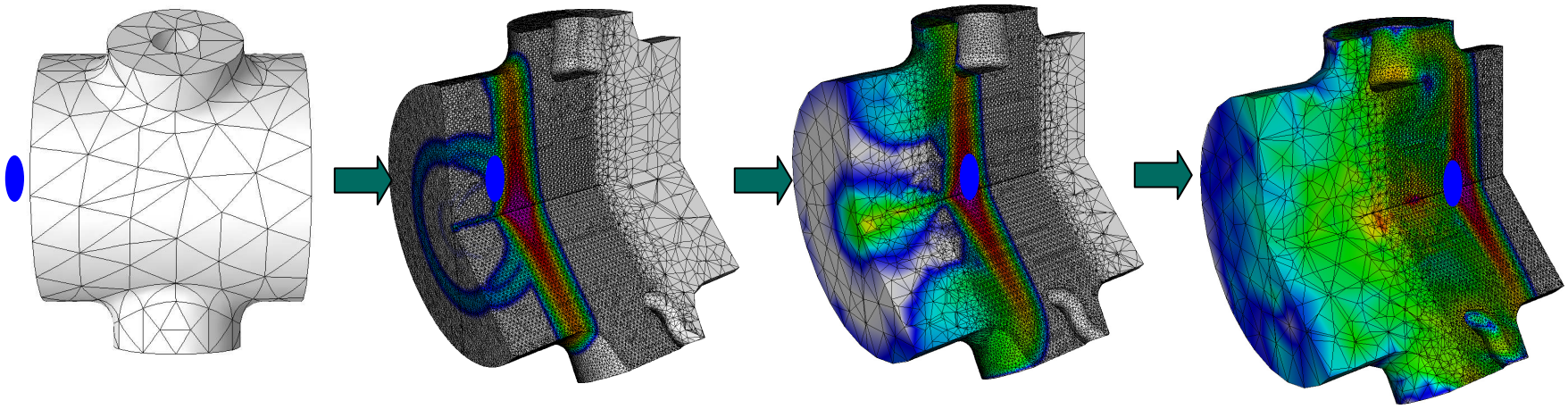




Moving Mesh Adaptation Examples

- FETD for short-range wakefield calculations
  - Adaptively refined meshes have **1~1.5** million curved regions
  - Uniform refined mesh using small mesh size has **6** million curved regions





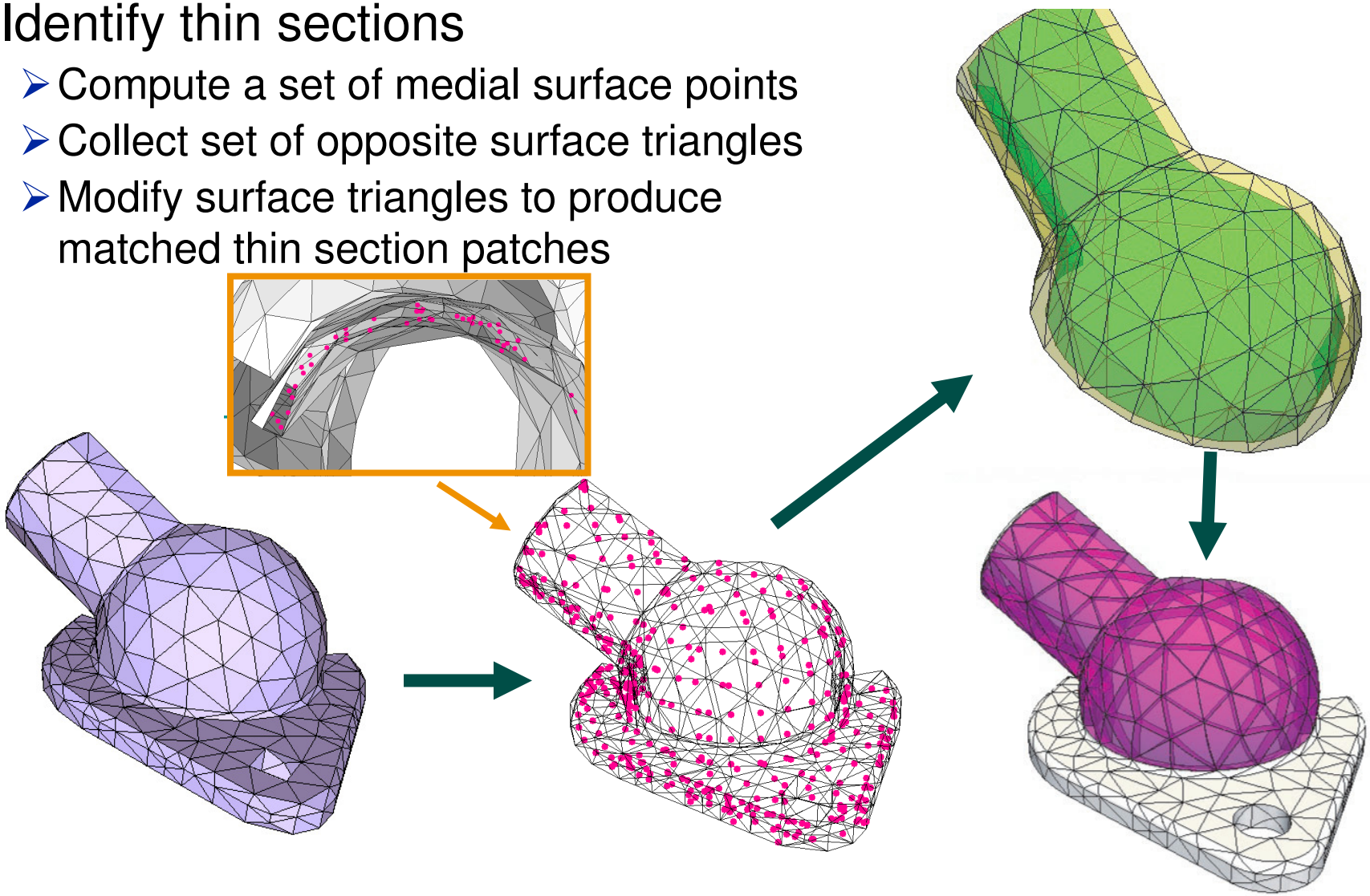
Electric fields on the three refined curved meshes

Curved Anisotropic Mesh Construction

- Input/Output
  - A CAD model with portions of thin domain as thin sections
  - A mesh with layered curved elements for thin sections and a tet mesh in the rest of the domains
- Procedure
  - Generate a curved surface mesh
  - Identify thin sections
  - Construct curved anisotropic layer elements for thin sections
  - Fill the rest of the domain with curved elements
- Key techniques
  - Automatically identify thin sections for complex geometry
  - Construct curved anisotropic layer elements with properly order

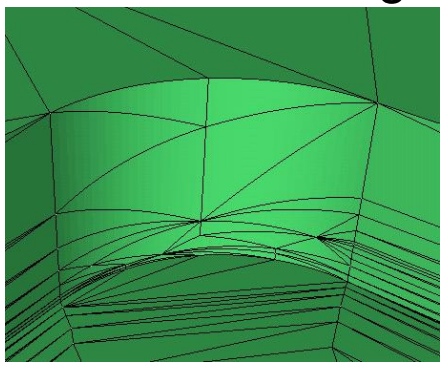
Identify Thin Sections

- Identify thin sections
  - Compute a set of medial surface points
  - Collect set of opposite surface triangles
  - Modify surface triangles to produce matched thin section patches

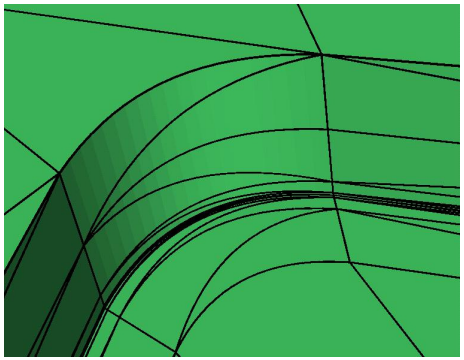


Construct Curved Anisotropic Elements

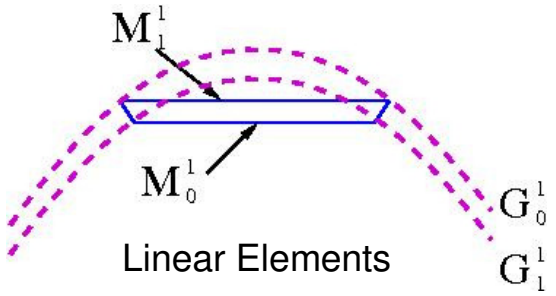
- Key techniques
  - Create layered prism elements by connecting matched pair triangles
  - Curve the prism elements in properly order
  - Split the prism elements into tetrahedral elements
  - Fill the remaining domains with unstructured tetrahedral elements



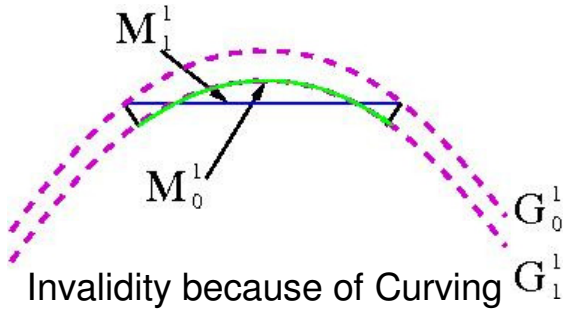
Curving without Gradation Control



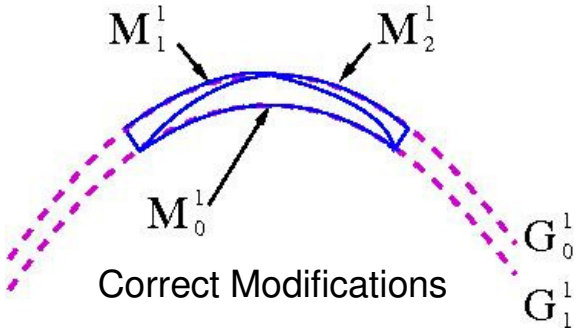
Curving with Gradation Control



Linear Elements

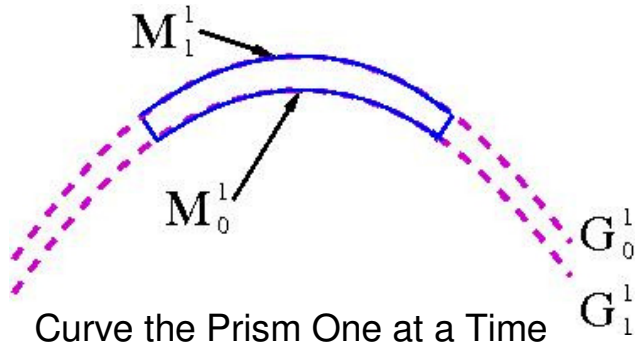


Invalidity because of Curving



Correct Modifications

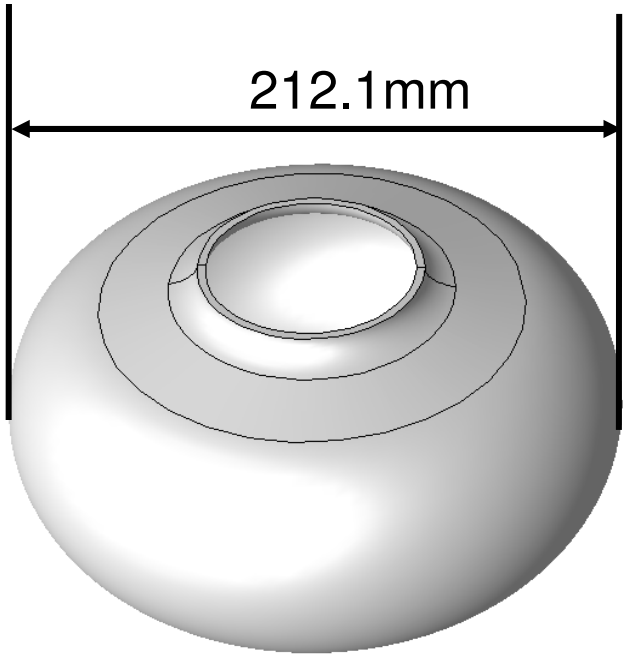
- **Not Desired**



Curve the Prism One at a Time

Application Examples of Curved Meshes

- Apply multi-physics analysis on 3D curved domains
  - Couple the electromagnetic, thermal/mechanical fields
  - Require 3 layer elements through the thin wall directions
  - Use coarse curved meshes along the models faces



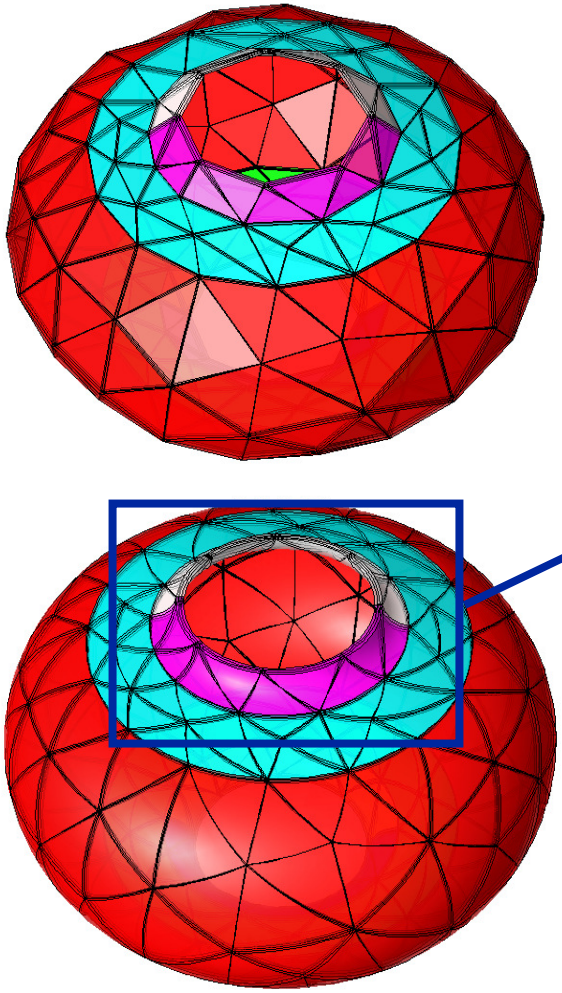
A cell model for the thermal/mechanical fields

Thickness: 2.98mm

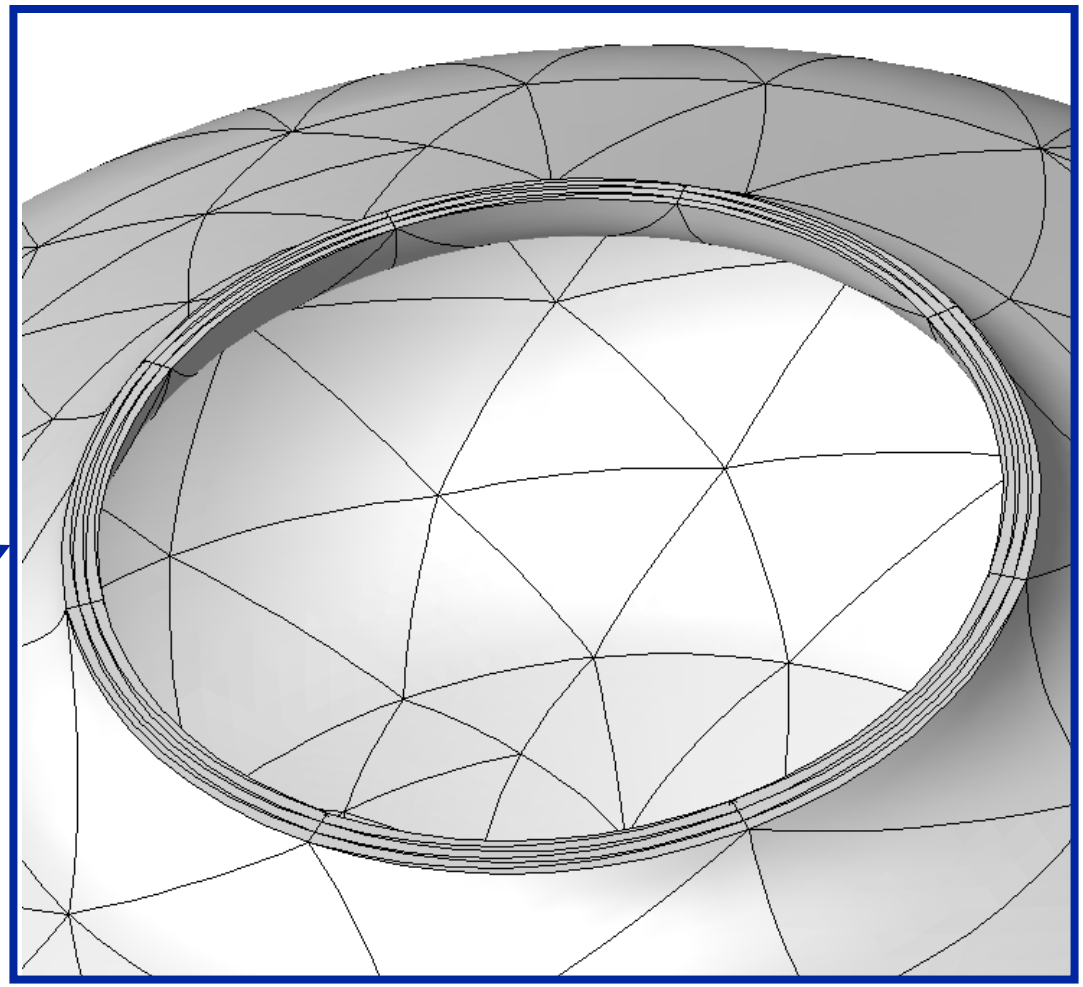
Height: 115.4mm

Curved Anisotropic Mesh Examples

2,664 tetrahedral regions

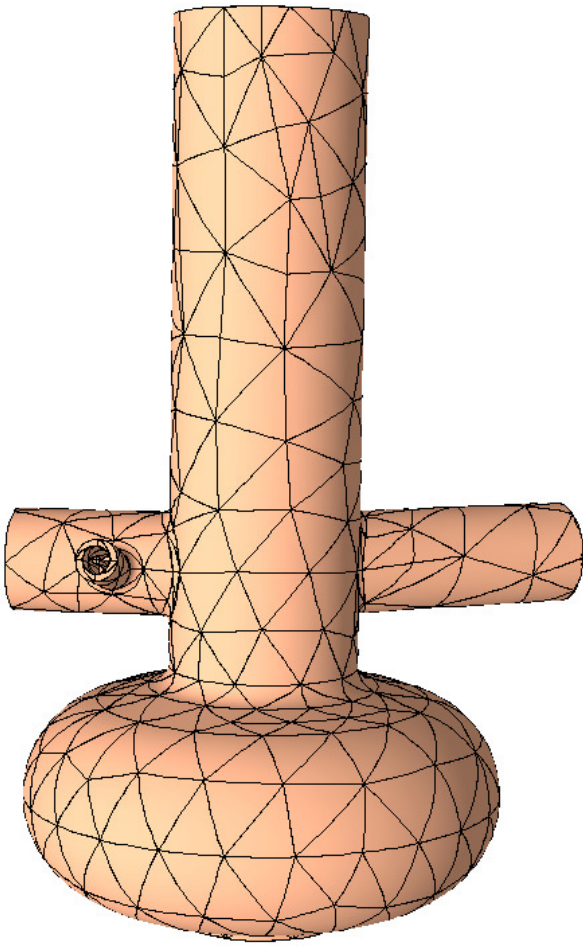


Straight-sided and curved anisotropic mesh for the cell model



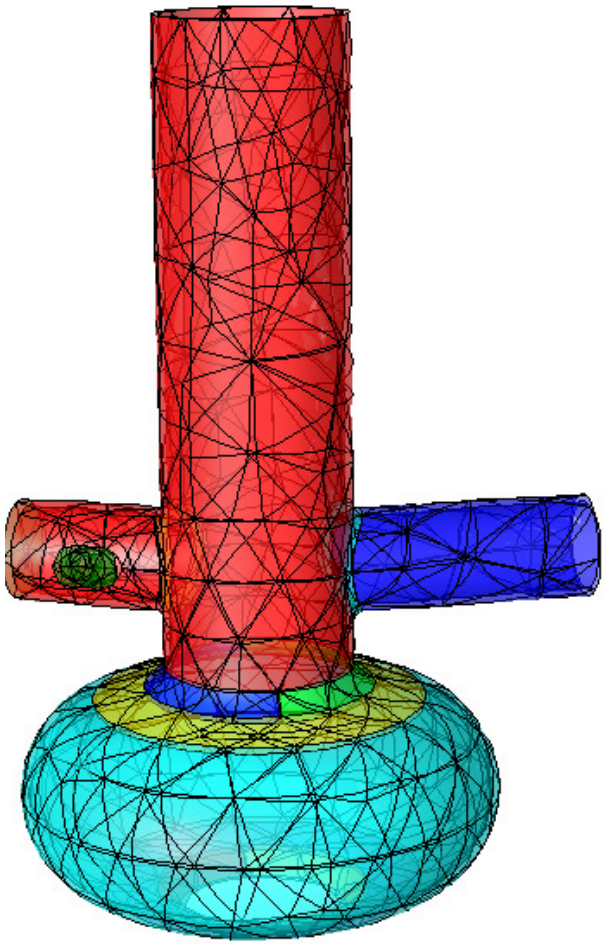
Close-up of the three curved layer elements on top of the model faces

Curved Anisotropic Mesh Examples



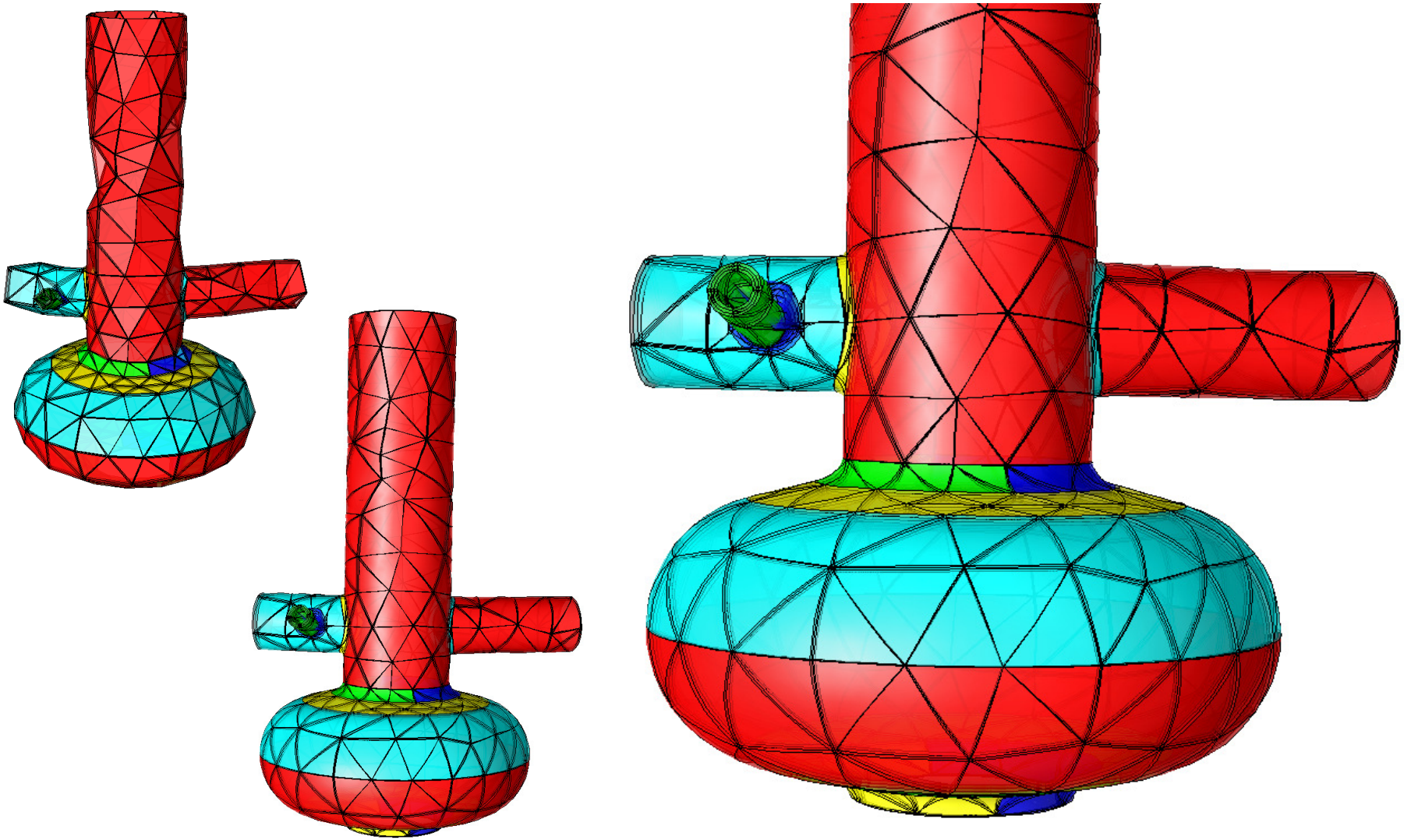
Curved surface mesh

Computed discrete medial surface points



Identified 14 thin sections out of 69 model faces

Curved Anisotropic Mesh Examples



Three layers for all of the identified thin sections

Conclusions

- Coordination Accomplishments
  - Developed stand alone mesh curving correction tool
  - Extended the mesh adaptation to deal with moving isotropic refinement in curvilinear mesh
  - Constructed curved anisotropic meshes for thin sections for thermal/mechanical multiphyscis simulations
  - Successfully applied to SLAC higher order electromagnetic simulations
- Future work
  - Provide effectively APIs to communicate with higher order solvers
    - Eliminate file I/O
    - Use ITAPS interfaces (iMesh, iGeom, iReln, iFeild, iMeshP ….)
  - High order solution field transfer
  - Additional work on thin section curved mesh creation
  - Parallelization